

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU011019\
 Data File : VU029110.D
 Acq On : 10 Jan 2019 11:50
 Operator : MD/SY
 Sample : K1094-01
 Misc : 2.70g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 CROSSWICKS-DRUM-1

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U010319W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.447	1296	1329	1369	rVB	3893194	10873566	10.23%	2.653%
2	9.254	2498	2513	2535	rBV	8910159	15253869	14.36%	3.722%
3	9.392	2536	2556	2568	rBV2	42437905	76597037	72.09%	18.690%
4	9.787	2663	2679	2709	rVB	21716897	35583637	33.49%	8.682%
5	10.591	2911	2929	2944	rBV	2801586	4388275	4.13%	1.071%
6	10.691	2944	2960	2977	rVV	17790445	42318127	39.83%	10.326%
7	10.781	2977	2988	3016	rVB	13665406	20457677	19.25%	4.992%
8	10.977	3033	3049	3070	rBV	12446294	19244297	18.11%	4.696%
9	11.173	3086	3110	3121	rBV3	56931049	106247634	100.00%	25.924%
10	11.430	3175	3190	3199	rBV	1385238	2144594	2.02%	0.523%
11	11.482	3199	3206	3219	rVB3	742631	1170531	1.10%	0.286%
12	11.578	3221	3236	3247	rBV	16292242	24767773	23.31%	6.043%
13	11.771	3282	3296	3303	rBV3	5609241	10353950	9.75%	2.526%
14	11.810	3303	3308	3317	rVV	5206743	7543616	7.10%	1.841%
15	11.877	3317	3329	3351	rVV3	6787560	13135957	12.36%	3.205%
16	12.057	3372	3385	3399	rVB	1577580	2354779	2.22%	0.575%
17	12.147	3399	3413	3418	rBV	3009038	4706025	4.43%	1.148%
18	12.176	3418	3422	3434	rVV	2471580	3360261	3.16%	0.820%
19	12.253	3434	3446	3468	rVV	4085355	6062436	5.71%	1.479%
20	12.649	3551	3569	3577	rBV	977163	1476566	1.39%	0.360%
21	12.700	3577	3585	3602	rVB	1214311	1796251	1.69%	0.438%

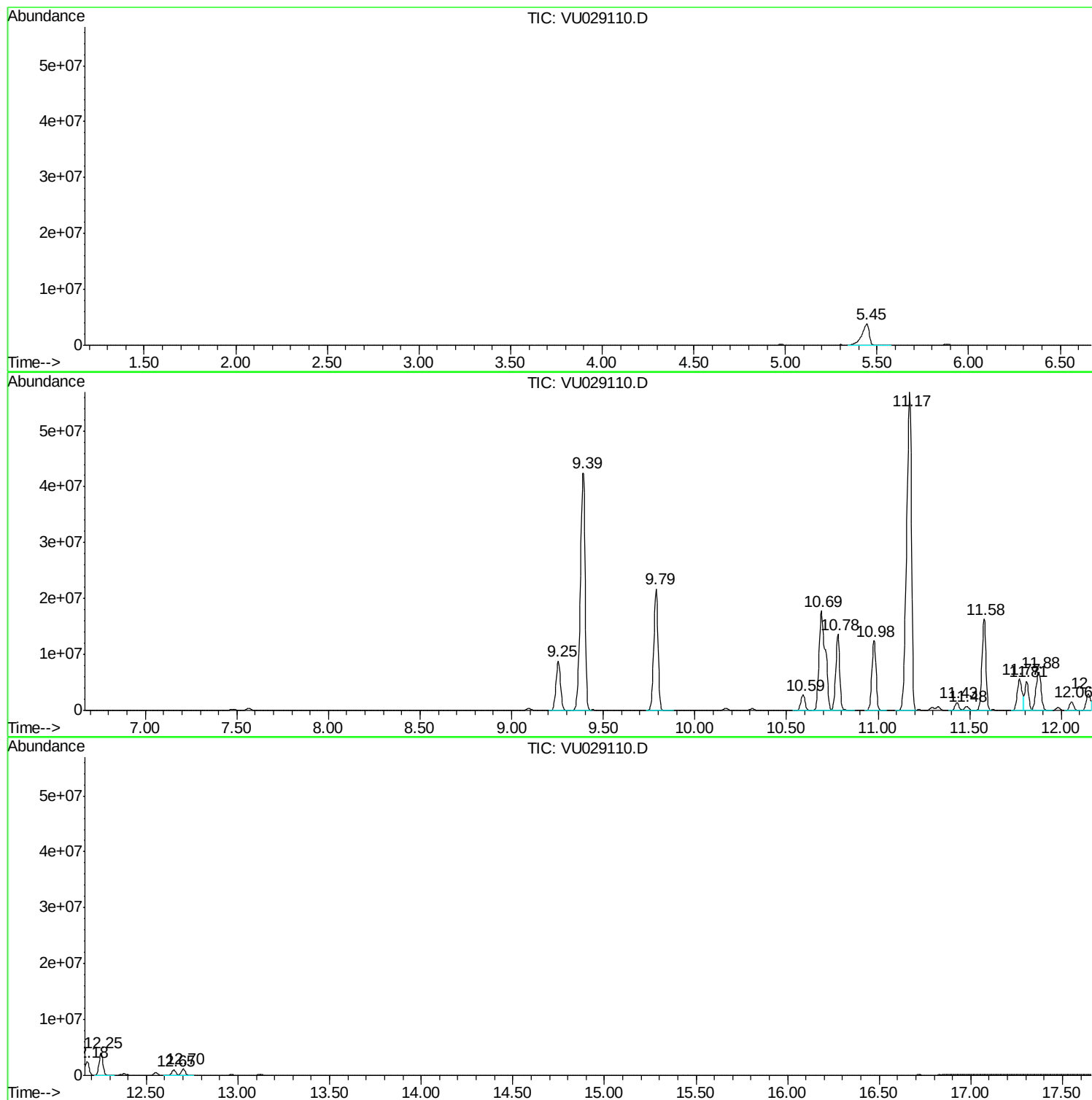
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CROSSWICKS-DRUM-1

Quant Method : Z:\HPCHEM1\MSVOA_U\METHOD\82U010319W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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ClientSampleId :
CROSSWICKS-DRUM-1

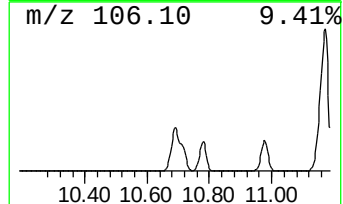
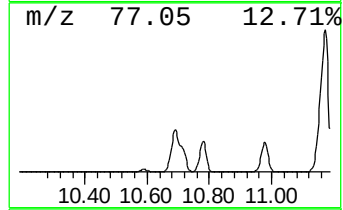
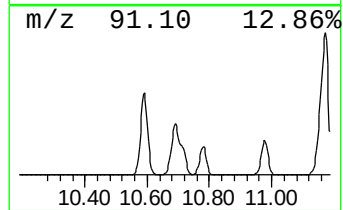
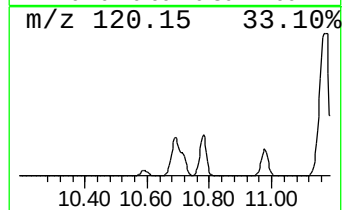
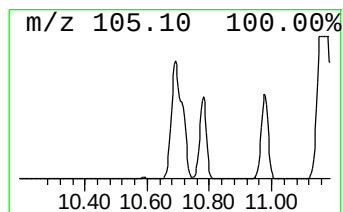
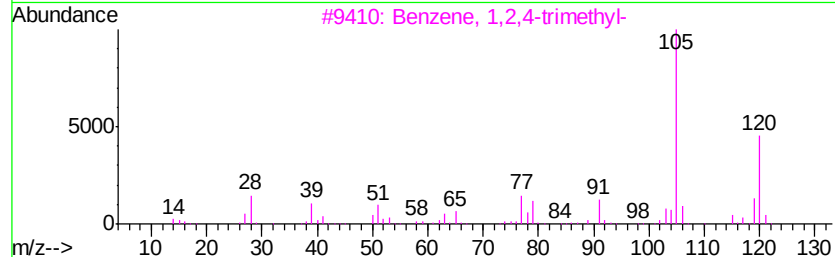
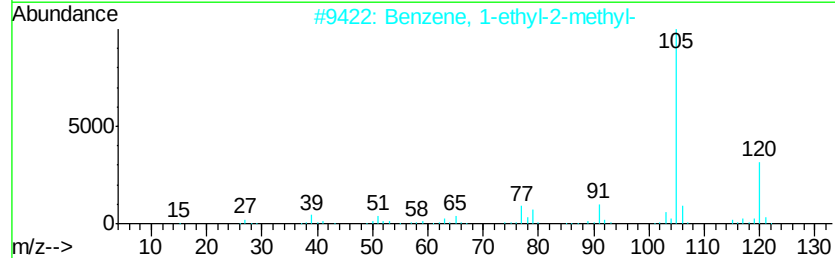
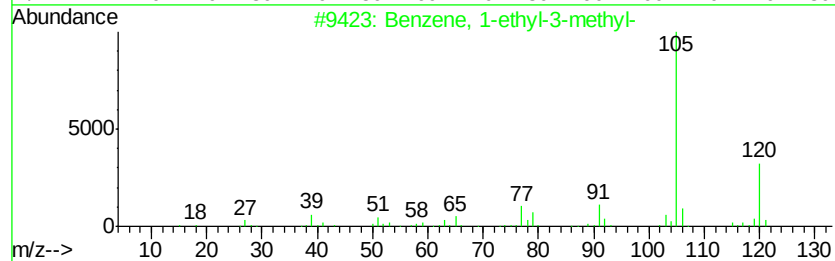
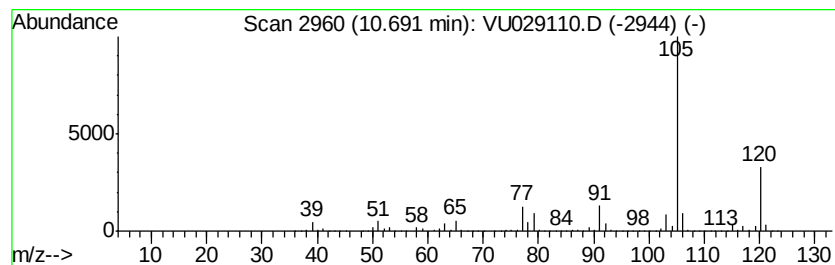
Quant Method : Z:\HPCHEM1\MSVOA_U\METHOD\82U010319W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Benzene, 1-ethyl-3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.69	1807.65 ug/l	42318100	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5		Mesitylene	120	C9H12	000108-67-8	91



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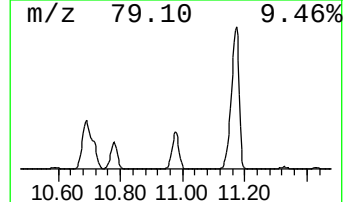
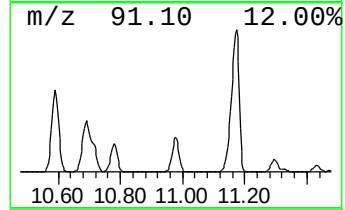
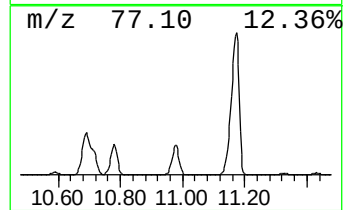
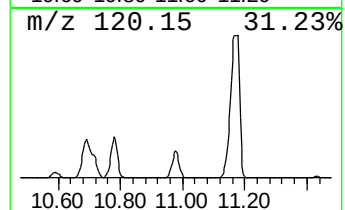
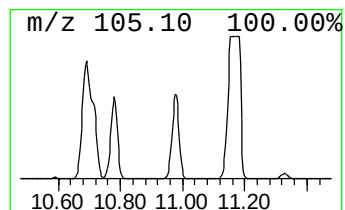
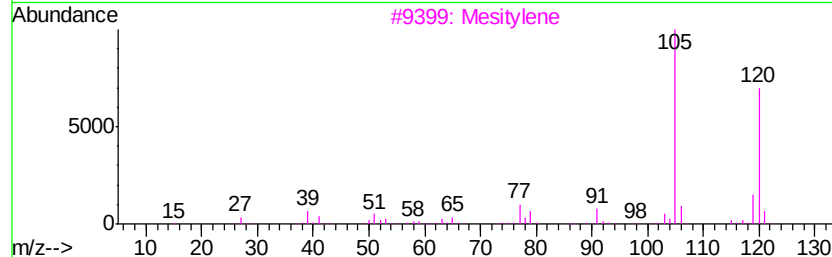
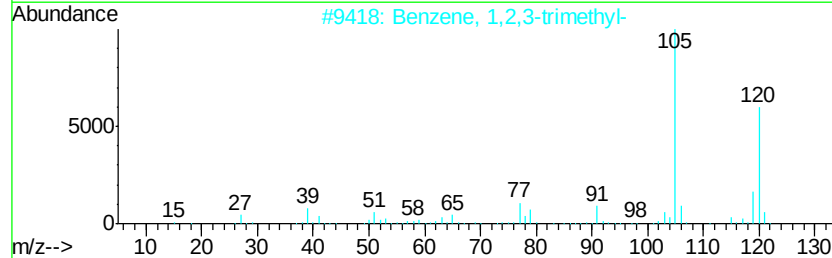
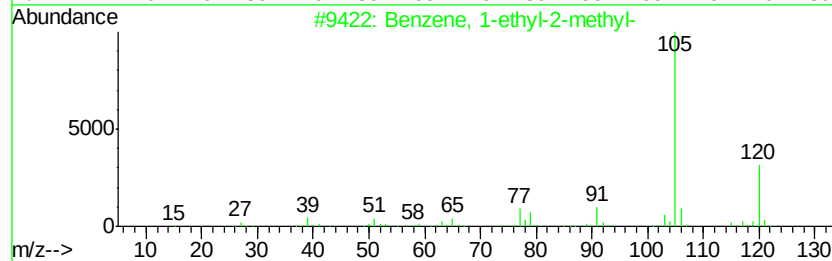
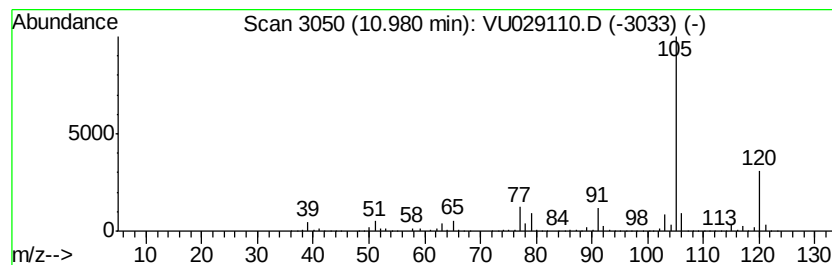
Instrument :
MSVOA_U
ClientSampleId :
CROSSWICKS-DRUM-1

Quant Method : Z:\HPCHEM1\MSVOA_U\METHOD\82U010319W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.98	822.03 ug/l	19244300	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 1-ethyl-2-methyl-	120 C9H12	000611-14-3 94
2		Benzene, 1,2,3-trimethyl-	120 C9H12	000526-73-8 91
3		Mesitylene	120 C9H12	000108-67-8 91
4		Benzene, 1,2,4-trimethyl-	120 C9H12	000095-63-6 91
5		Benzene, 1-ethyl-4-methyl-	120 C9H12	000622-96-8 91



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ALS Vial : 8 Sample Multiplier: 1

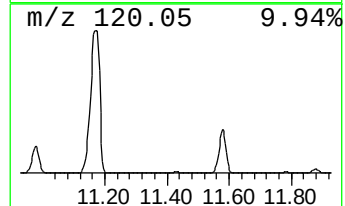
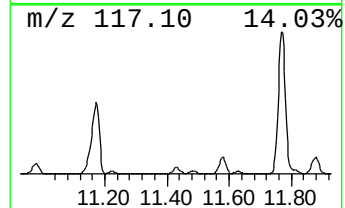
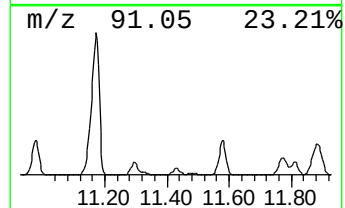
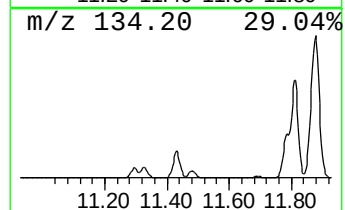
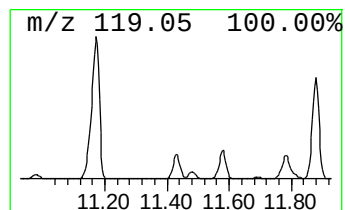
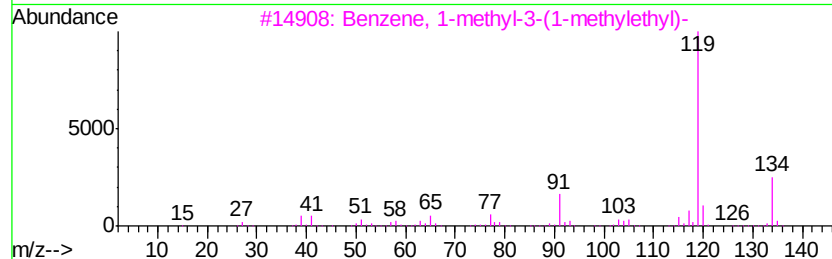
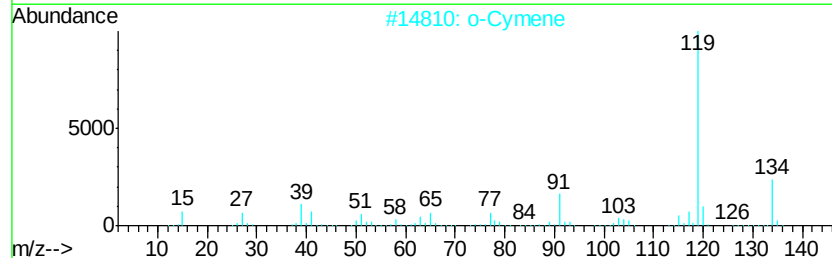
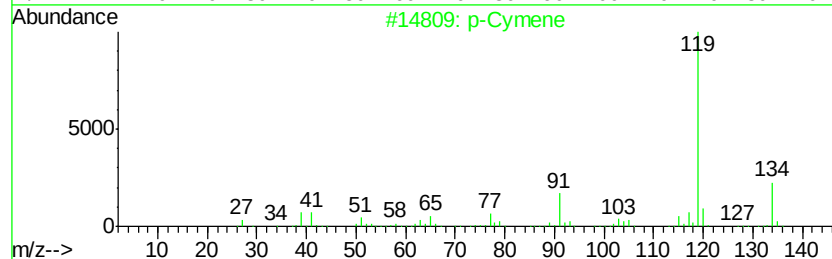
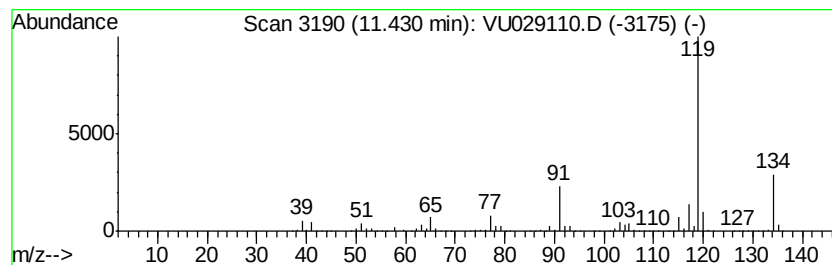
Instrument :
MSVOA_U
ClientSampleId :
CROSSWICKS-DRUM-1

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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 p-Cymene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	91.61 ug/l	2144590	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	p-Cymene	134 C10H14	000099-87-6	97
2	o-Cymene	134 C10H14	000527-84-4	97
3	Benzene, 1-methyl-3-(1-methylethyl)-	134 C10H14	000535-77-3	95
4	Benzene, 4-ethyl-1,2-dimethyl-	134 C10H14	000934-80-5	91
5	Benzene, 1-ethyl-2,3-dimethyl-	134 C10H14	000933-98-2	91



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Sample : K1094-01
Misc : 2.70uL/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
CROSSWICKS-DRUM-1

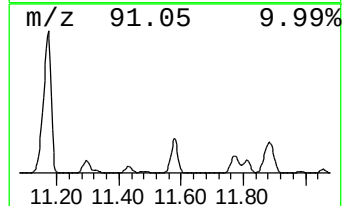
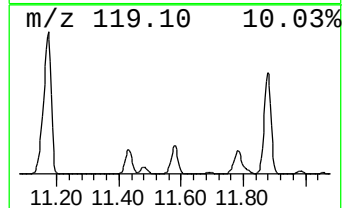
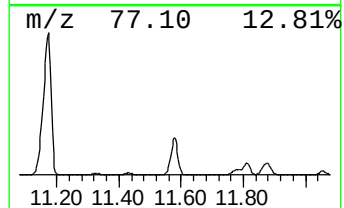
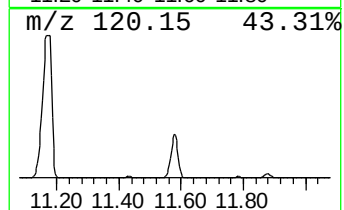
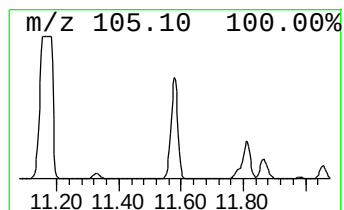
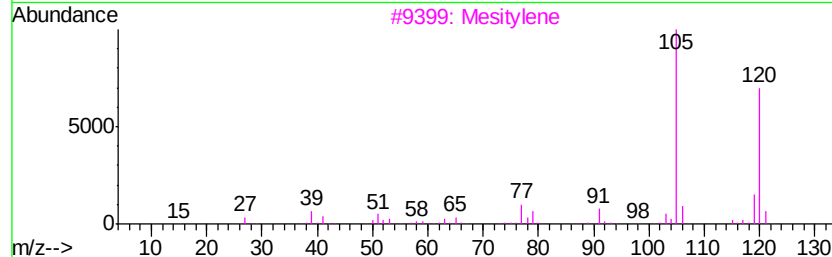
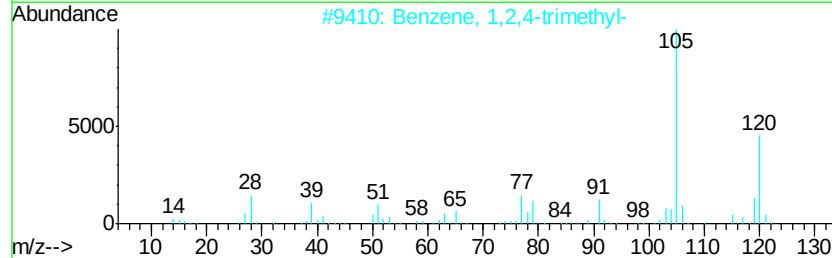
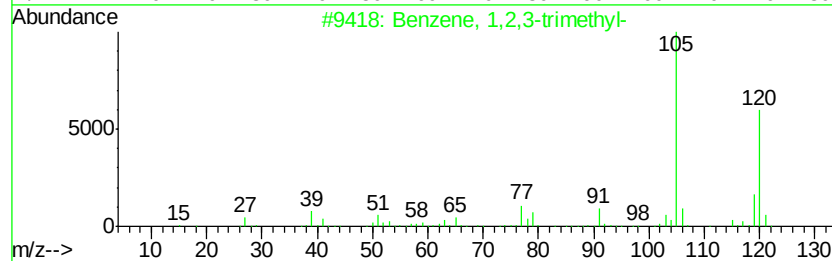
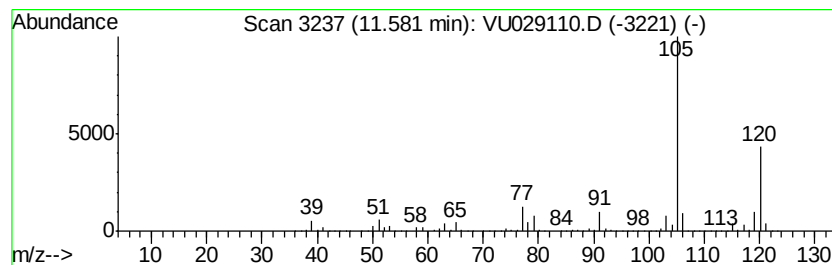
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1,2,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.58	1057.97 ug/l	24767800	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
3		Mesitylene	120	C9H12	000108-67-8	91
4		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90



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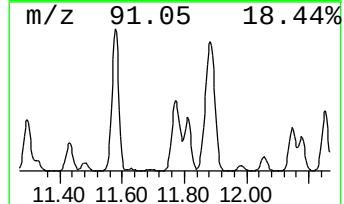
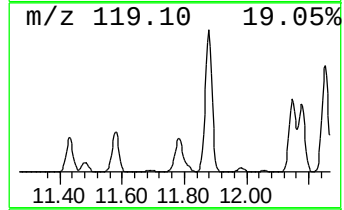
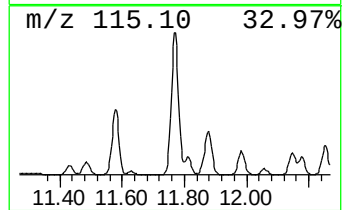
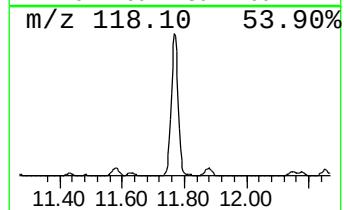
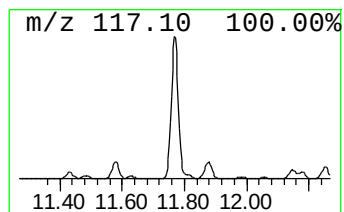
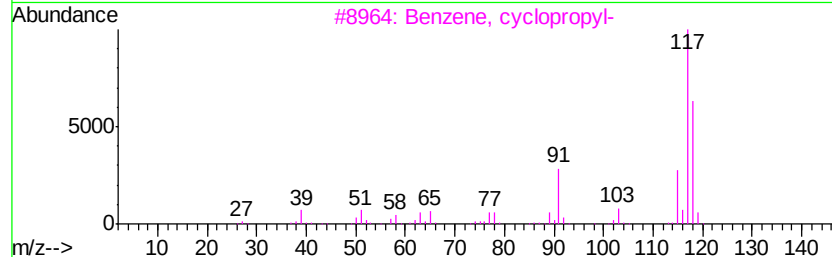
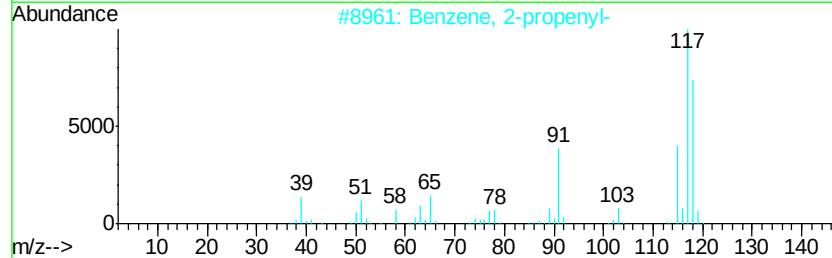
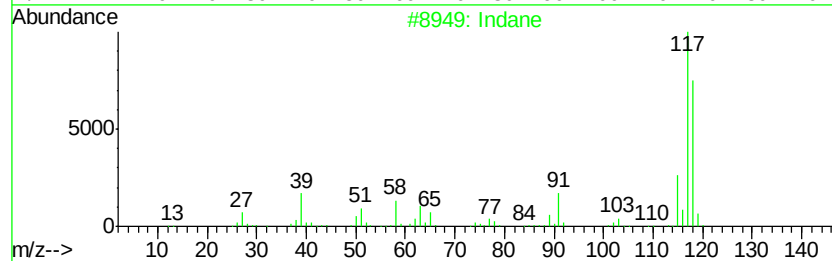
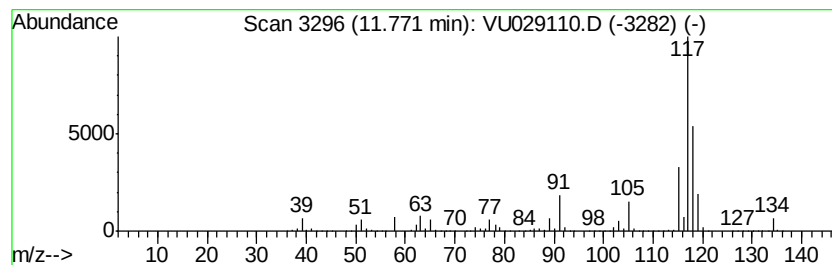
Instrument :
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.77	442.28 ug/l	10354000	1,4-Dichlorobenzene-d4	11.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	76
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
3	Benzene, cvclopropvl-	118	C9H10	000873-49-4	76
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	55
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	53



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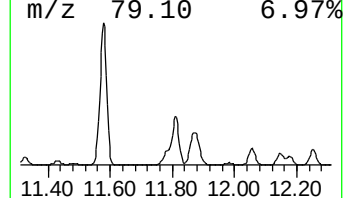
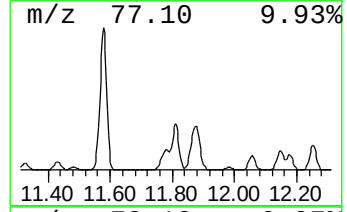
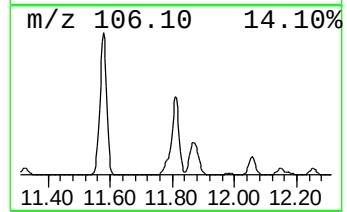
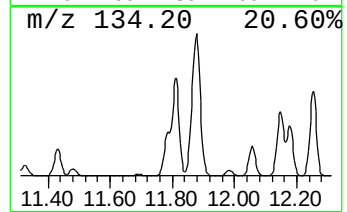
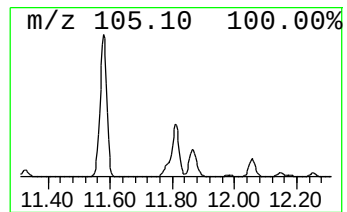
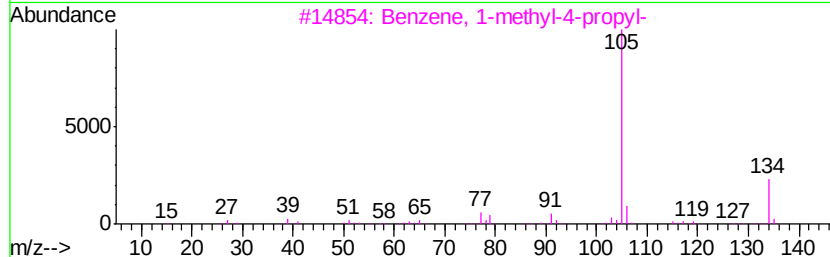
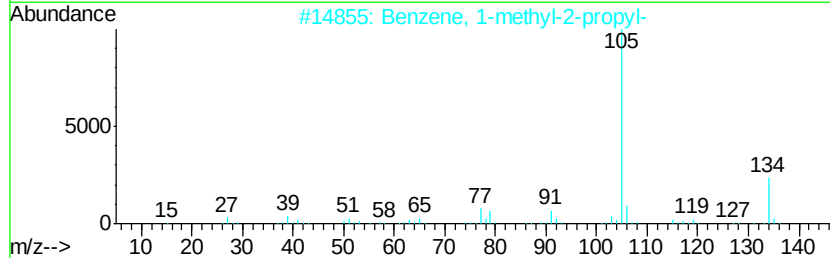
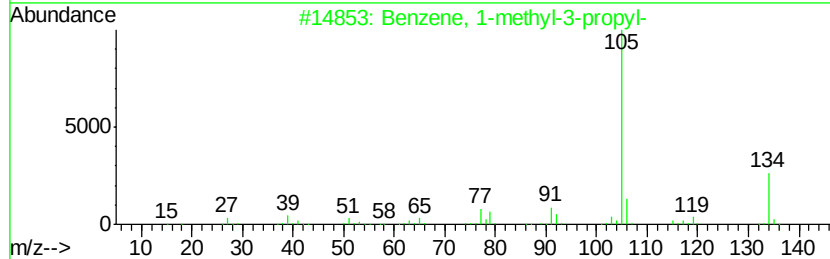
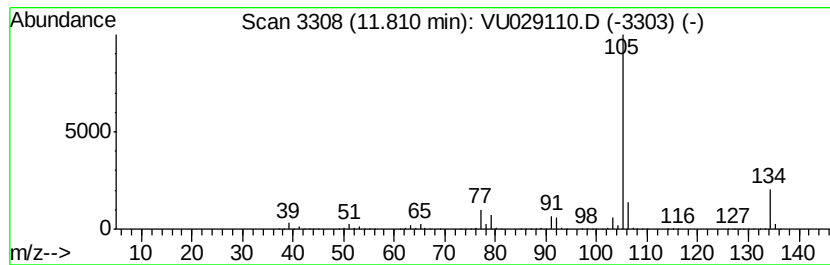
Instrument :
MSVOA_U
ClientSampleId :
CROSSWICKS-DRUM-1

Quant Method : Z:\HPCHEM1\MSVOA_U\METHOD\82U010319W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzene, 1-methyl-3-propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.81	322.23 ug/l	7543620	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 1-methyl-3-propyl-	134 C10H14	001074-43-7 91
2		Benzene, 1-methyl-2-propyl-	134 C10H14	001074-17-5 91
3		Benzene, 1-methyl-4-propyl-	134 C10H14	001074-55-1 91
4		Benzene, (1-methylpropyl)-	134 C10H14	000135-98-8 72
5		2-Indanol	134 C9H10O	004254-29-9 72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU011019\
Data File : VU029110.D
Acq On : 10 Jan 2019 11:50
Operator : MD/SY
Sample : K1094-01
Misc : 2.70µ/5mL/100µL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
CROSSWICKS-DRUM-1

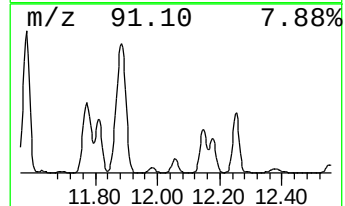
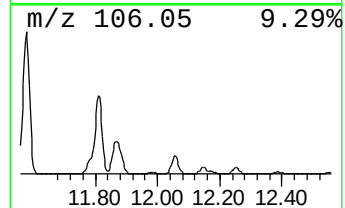
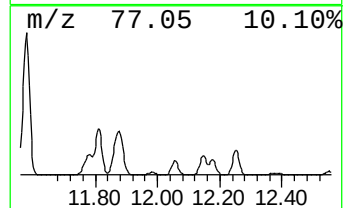
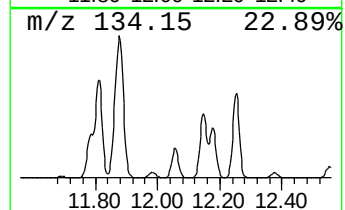
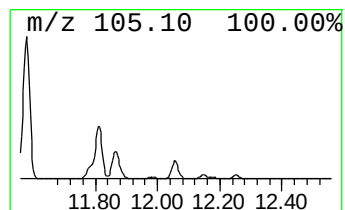
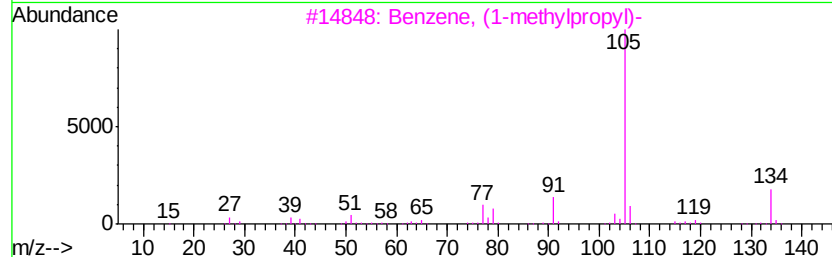
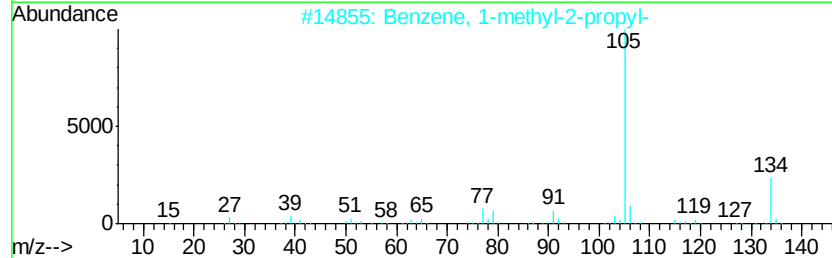
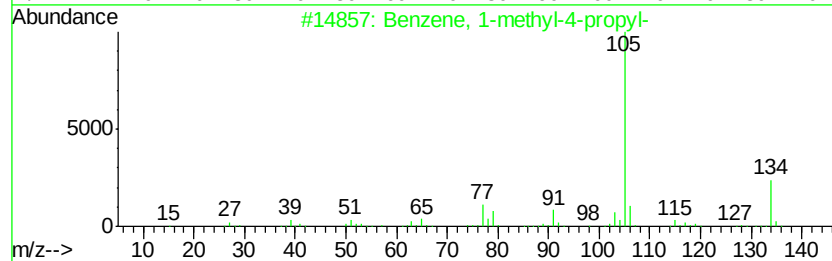
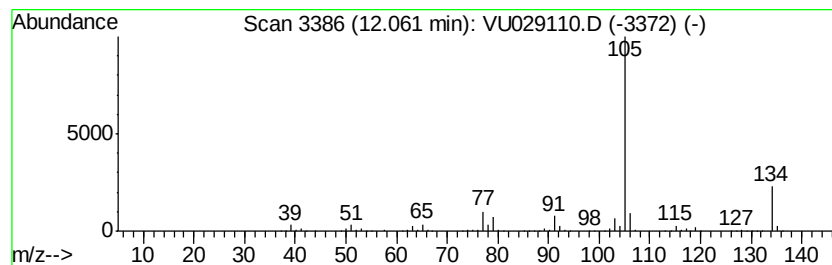
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzene, 1-methyl-4-propyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.06	100.59 ug/l	2354780	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	95
2		Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	94
3		Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	91
4		Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	90
5		Benzeneacetaldehyde, .alpha.-met...	134	C9H10O	000093-53-8	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU011019\
Data File : VU029110.D
Acq On : 10 Jan 2019 11:50
Operator : MD/SY
Sample : K1094-01
Misc : 2.70µL/5mL/100µL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
CROSSWICKS-DRUM-1

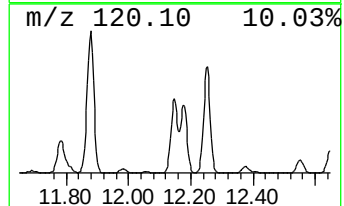
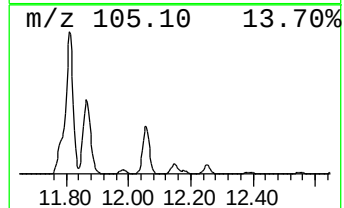
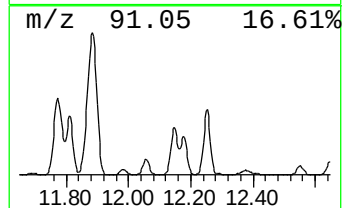
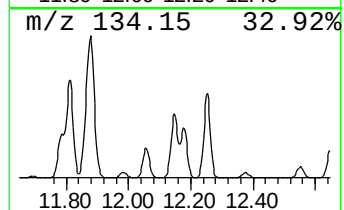
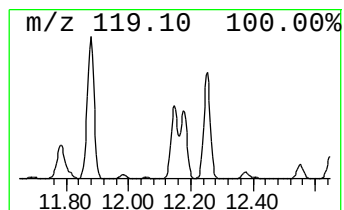
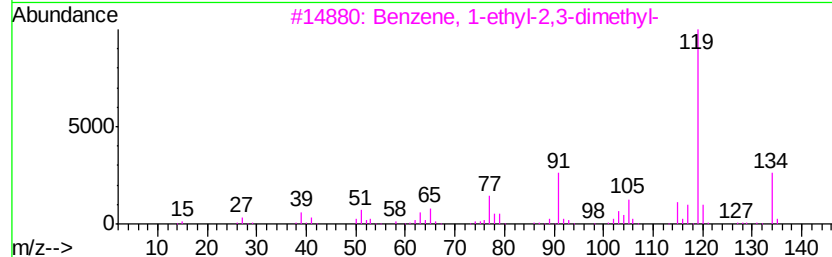
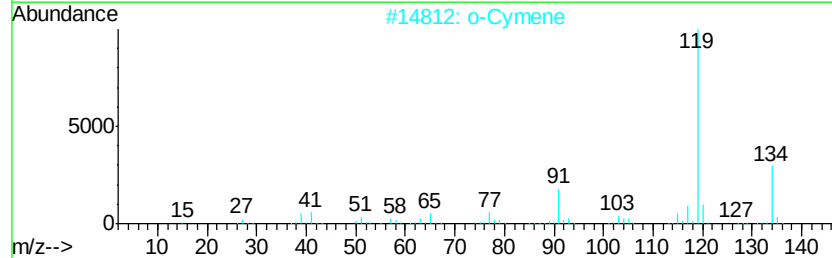
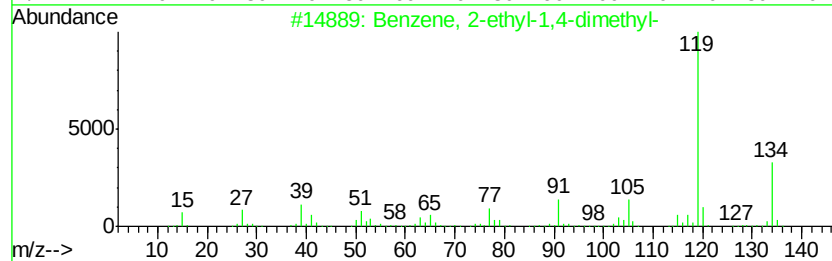
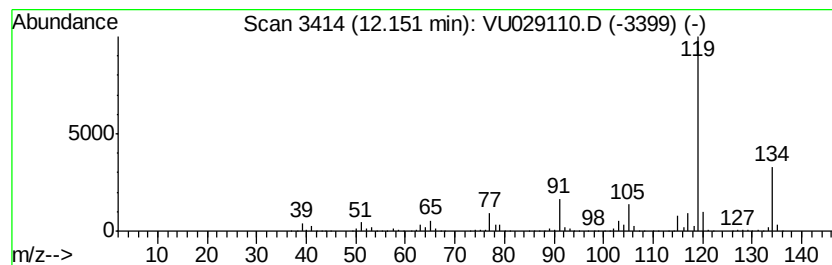
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.15	201.02 ug/l	4706030	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	97
2		o-Cymene	134	C10H14	000527-84-4	95
3		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4		Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
5		Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU011019\
Data File : VU029110.D
Acq On : 10 Jan 2019 11:50
Operator : MD/SY
Sample : K1094-01
Misc : 2.70uL/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
CROSSWICKS-DRUM-1

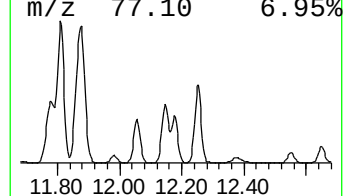
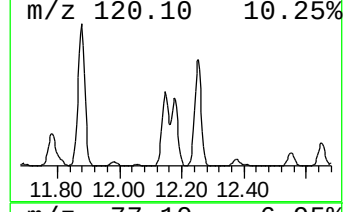
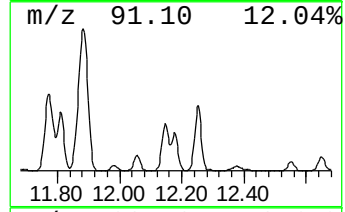
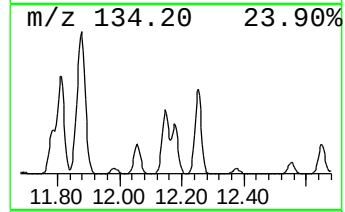
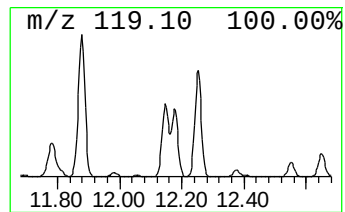
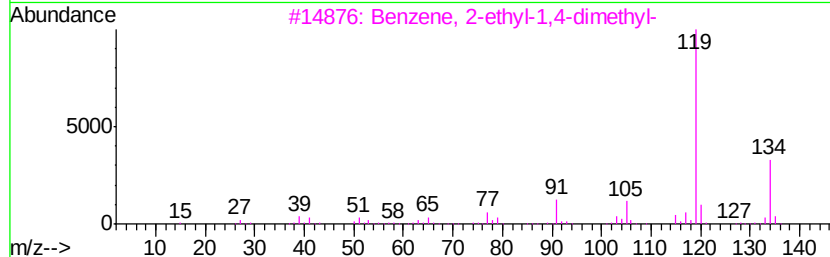
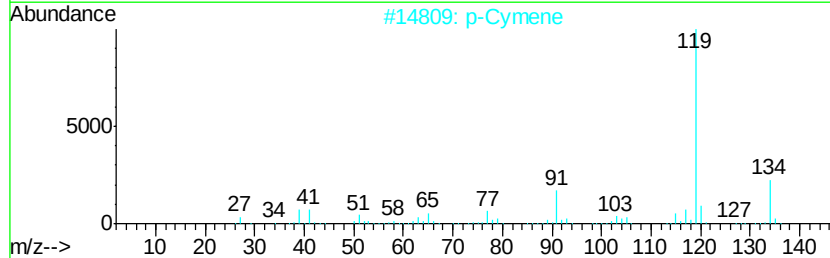
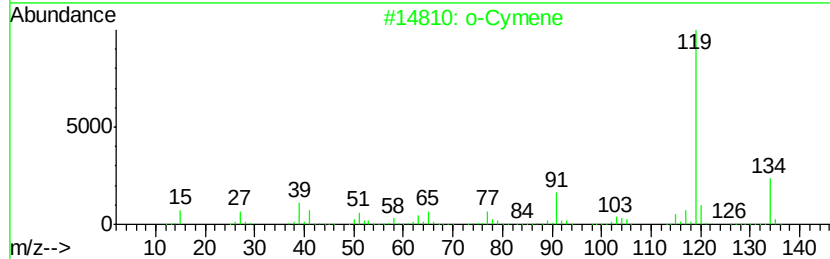
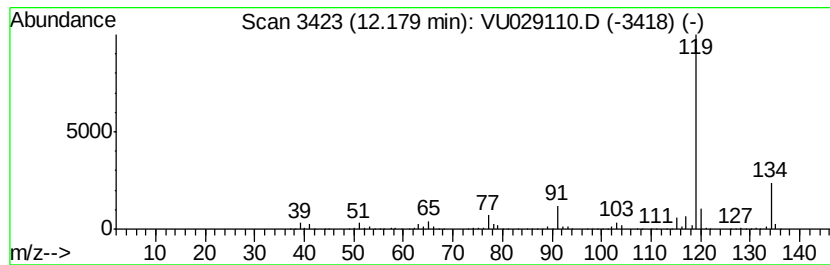
Quant Method : Z:\HPCHEM1\MSVOA_U\METHOD\82U010319W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 o-Cymene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.18	143.54 ug/l	3360260	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	o-Cymene	134	C10H14	000527-84-4	94
2		p-Cymene	134	C10H14	000099-87-6	94
3		Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	91
4		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	91
5		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU011019\
Data File : VU029110.D
Acq On : 10 Jan 2019 11:50
Operator : MD/SY
Sample : K1094-01
Misc : 2.70uL/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
CROSSWICKS-DRUM-1

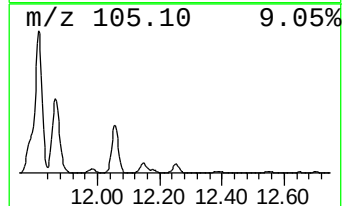
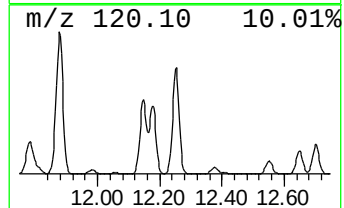
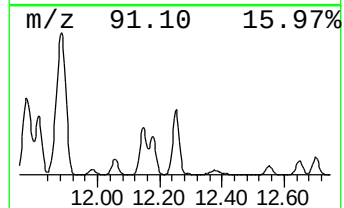
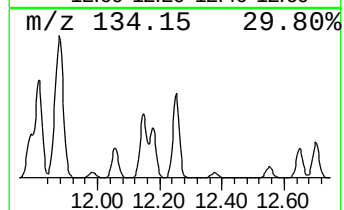
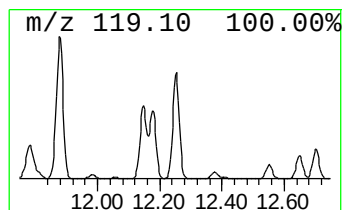
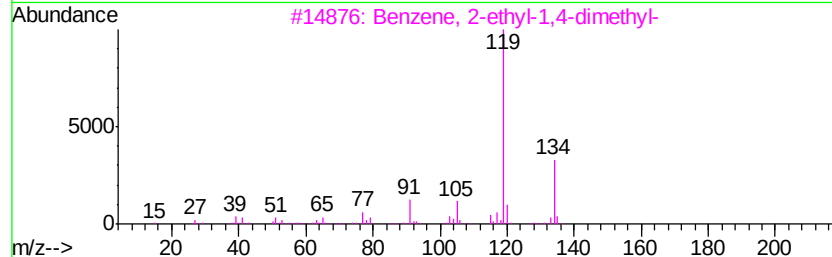
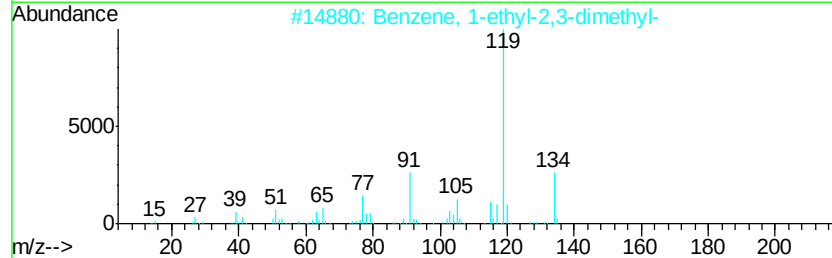
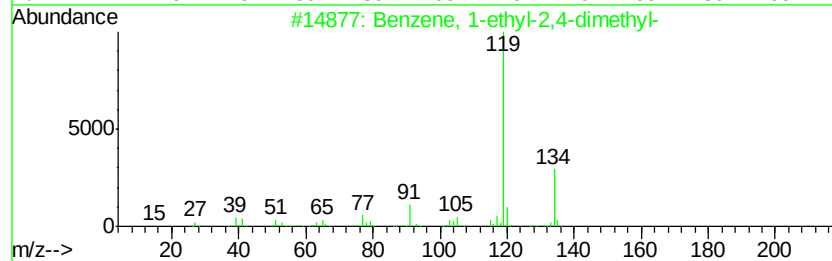
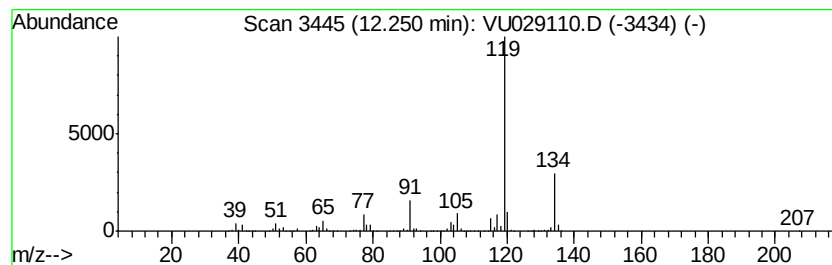
Quant Method : Z:\HPCHEM1\MSVOA_U\METHOD\82U010319W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.25	258.96 ug/l	6062440	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
3		Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
4		Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
5		Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU011019\
 Data File : VU029110.D
 Acq On : 10 Jan 2019 11:50
 Operator : MD/SY
 Sample : K1094-01
 Misc : 2.70g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 CROSSWICKS-DRUM-1

Quant Method : Z:\HPCHEM1\MSVOA_U\METHOD\82U010319W.M
 Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1-ethyl-...	10.69	1807.7	ug/l	42318100	4	11.48	1170530	50.0
Benzene, 1-ethyl-...	10.98	822.0	ug/l	19244300	4	11.48	1170530	50.0
p-Cymene	11.43	91.6	ug/l	2144590	4	11.48	1170530	50.0
Benzene, 1,2,3-tr...	11.58	1058.0	ug/l	24767800	4	11.48	1170530	50.0
Indane	11.77	442.3	ug/l	10354000	4	11.48	1170530	50.0
Benzene, 1-methyl...	11.81	322.2	ug/l	7543620	4	11.48	1170530	50.0
Benzene, 1-methyl...	12.06	100.6	ug/l	2354780	4	11.48	1170530	50.0
Benzene, 2-ethyl-...	12.15	201.0	ug/l	4706030	4	11.48	1170530	50.0
o-Cymene	12.18	143.5	ug/l	3360260	4	11.48	1170530	50.0
Benzene, 1-ethyl-...	12.25	259.0	ug/l	6062440	4	11.48	1170530	50.0